

Fluctuations in Hertz chains at equilibrium

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We examine the long-term behavior of nonintegrable, energy-conserved, one-dimensional systems of macroscopic grains interacting via a contact-only generalized Hertz potential and held between stationary walls. Such systems can be set up to have no phononic background excitation and represent examples of a sonic vacuum. Existing dynamical studies showed the absence of energy equipartitioning in such systems, hence their long-term dynamics was described as *quasiequilibrium*. Here we show that these systems do in fact reach thermal equilibrium at sufficiently long times, as indicated by the calculated heat capacity. As a by-product, we show how fluctuations of system quantities, and thus the distribution functions, are influenced by the Hertz potential. In particular, the variance of the system's kinetic energy probability density function is reduced by a factor related to the contact potential.

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I. INTRODUCTION

Recently, there has been broad interest in one-dimensional (1D) systems of macroscopic grains held between stationary walls and interacting via a power-law contact potential [1–7]. A long-standing open problem is whether thermalization (equipartition) can occur in these chains of grains. Only very recently has it been shown that the related Fermi-Pasta-Ulam (FPU) chain of coupled oscillators does reach equilibrium after very long times [8]. In this paper, we show this is also true for so-called Hertz chains. In the process, we obtain wholly different approximate distribution functions for *interacting* particles in the *microcanonical* ensemble.

Many power-law interacting systems are notable for supporting solitary wave (SW) propagation [7,3,9]. However, in response to singular perturbations, the breakup of SWs at the walls and from gaps between grains leads the system after a long time to an equilibriumlike, ergodic phase [2–4]. Unusually large [2–4] and occasionally persistent (rogue) [10] fluctuations in the system's kinetic energy are seen at late times for sufficiently strong and unique perturbations. This has been seen to impede an equal sharing of energy among all the grains in the system, hence the long-term dynamics of 1D systems of interacting grains has been described as quasiequilibrium (QEQ) [2–4]. The question of whether QEQ is the final state for such systems excited by gentle point perturbations is addressed in this paper.

To the time scales previously studied, quasiequilibrium has been seen to be a general feature of the dynamics of systems with no sound propagation [3]. However, we find in our studies that at sufficiently late times, kinetic energy fluctuations relax, allowing for energy to be shared equally among all grains. Of course, energy equipartitioning happens only in an average sense in finite systems, and at any given instant each grain will not have exactly the same kinetic energy. Rather, each grain's kinetic energy fluctuates according to the same probability density function (pdf), the long tail of which determines the chance of large fluctuations.

The fluctuations are quantified by treating the chain as a 1D gas of interacting spheres [11]. This requires velocity and kinetic energy distribution functions that are different

from hard spheres, which incorporate the interaction potential. These distributions are also influenced by the finite heat capacity of the system, which governs the fluctuations in the system kinetic energy in a microcanonical ensemble [12]. An equilibrium value for the specific heat obtained using Tolman's generalized equipartition theorem [13] provides a direct way to probe the extent to which energy equipartitioning occurs in large but finite systems. We show that at sufficiently long times, calculated specific heat capacities of chains of interacting grains agree with the values predicted by the generalized equipartition theorem, indicating that energy equipartitioning holds, and consequently that the ultimate fate of these systems is a true equilibrium phase that can be described by statistical mechanics.

The paper is organized as follows. In Sec. II we introduce the model for the Hertz chains and use the machinery of equilibrium statistical mechanics to derive the expected equilibrium value of the heat capacity and the approximate distribution functions. Then we give the details of the numerical simulations in Sec. III. In Sec. IV we compare molecular dynamics (MD) data with the predicted equilibrium values to establish that our systems do equilibrate at long times. Finally, we give some concluding remarks and discuss future research directions in Sec. V.

II. MODEL AND THEORETICAL BACKGROUND

The specific systems under consideration are 1D chains of N grains, each with mass m and radius R , interacting via a Hertz-like contact-only potential [14]. The Hamiltonian describing the system is

$$H = K + U = \frac{1}{2} \sum_{i=1}^N m v_i^2 + \sum_{i=1}^{N-1} a \Delta_{i,i+1}^n, \quad (1)$$

where v_i is the velocity of grain i and $\Delta_{i,i+1} \equiv 2R - (x_{i+1} - x_i) \geq 0$ is the overlap between neighboring grains, located at position x_i . There is no potential interaction when the grains are not in contact. In the above expression, the exponent n is shape dependent ($n = 2.5$ for spheres), and a contains the material properties and radius of curvature of the grains [15].

The grain interactions with the fixed walls add two terms to the Hamiltonian. In particular, the walls are implemented by taking the limit $R \rightarrow \infty$ as the radius of the wall, which ensures that the boundary is much larger than any grain in the chain and will therefore not move, while also relaxing the condition that the wall must be flat [7]. In this way, the prefactor a in the potential energy describing grain-wall interactions is then a factor of $\sqrt{2}$ larger than the grain-grain interaction potential prefactor.

The total system energy is taken to be fixed, $H = \text{const} = E$. Since our primary aim is to establish that the systems under consideration are described by a microcanonical ensemble of interacting particles long after an initial energy perturbation, we now discuss the relevant theoretical background.

The pdf of particle velocity of a d -dimensional, finite sized microcanonical ensemble is not a Maxwell-Boltzmann distribution [11,16]. The actual distribution can be found from the total volume of a $2dN$ -dimensional phase space circumscribed by the total energy E ,

$$\Omega \propto \int \Theta(E - H) dq^{dN} dp^{dN}, \quad (2)$$

where Θ is the Heaviside step function. The integral in Eq. (2) is taken over all grain momenta \mathbf{p} and all grain positions \mathbf{q} . Integration over the grain momenta evaluates to the volume of a dN -dimensional hypersphere of radius $[2m(E - U)]^{1/2}$, leaving the remaining integral over the grain positions:

$$\Omega \propto \int (E - U)^{dN/2} \Theta(E - U) dq^{dN}. \quad (3)$$

This integral has been evaluated analytically for hard spheres, where the system potential energy $U = 0$ [11,16,17], but to the best of our knowledge, not for any case of an interaction potential.

Indeed, there may not be an exact analytic solution for the Hamiltonian in Eq. (1). Instead, we seek an approximate solution, and making the simple observation that the virial theorem holds for these systems, replace $(E - U)$ with $(E - \langle U \rangle_v) = \langle K \rangle_v$, where $\langle \dots \rangle_v$ denotes the expected value from the virial theorem. For Eq. (1), the virial theorem yields $2\langle K \rangle_v = n\langle U \rangle_v$, and thus

$$\frac{\langle U \rangle_v}{E} = \frac{2}{n+2}, \quad \frac{\langle K \rangle_v}{E} = \frac{n}{n+2}, \quad (4)$$

with K the system kinetic energy. Thus $\langle K \rangle_v$ can come out of the integral in Eq. (3), and the integral proceeds as previously described [11,16,17].

This substitution cannot be exact: The grain momentum's limit is now set by $\langle K \rangle_v$, an *average* value, and there are certainly grains with kinetic energy that, at times, are slightly greater than this value. However, we can rely on decreasing fluctuations with increasing N , and show that for $N > 10$, the number of states beyond this limit is small, and this is a very good approximation.

The resulting pdf of per-grain velocities v_i in 1D is then [11]

$$\begin{aligned} \text{pdf}(v_i) &= \text{B}(\alpha, \beta, \tilde{v}_i) / (2\langle v \rangle_v), \\ &= \frac{1}{2\langle v \rangle_v} \left(\frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} (\tilde{v}_i)^{\alpha-1} (1 - \tilde{v}_i)^{\beta-1} \right), \end{aligned} \quad (5)$$

where

$$\tilde{v}_i = \frac{1}{2} \left(1 - \frac{v_i}{\langle v \rangle_v} \right), \quad (6)$$

with $\langle v \rangle_v^2 = 2\langle K \rangle_v/m$, and $\alpha = \beta = (N - 1)/2$. Also, $\text{B}(\alpha, \beta, \tilde{v}_i)$ is the beta distribution, and Γ is the gamma function. In the limit $N \gg 1$, Eq. (5) becomes the familiar Maxwell-Boltzmann 1D normal distribution with mean $\mu = 0$ and variance $\sigma^2 = \langle v \rangle_v^2/N$.

The distribution of kinetic energy per grain K_i is also given by a beta distribution [11],

$$\text{pdf}(K_i) = \text{B}(\alpha, \beta; \tilde{K}) / \langle K \rangle_v, \quad (7)$$

where $\tilde{K} = K_i / \langle K \rangle_v$, $\alpha = 1/2$, and $\beta = (N - 1)/2$. For $N \gg 1$, this becomes the familiar Maxwell-Boltzmann distribution for kinetic energy, a gamma distribution $\text{G}(\alpha, \beta, K_i)$,

$$\text{pdf}(K_i) = \text{G}(\alpha, \beta, K_i) = \frac{\beta^\alpha}{\Gamma(\alpha)} K_i^{\alpha-1} e^{-\beta K_i}, \quad (8)$$

where $\alpha = 1/2$ and $\beta = N/(2\langle K \rangle_v)$. Interestingly, the possibility of large kinetic energy fluctuations increases with the variance of Eq. (7) [and Eq. (8)], $\langle \delta K_i^2 \rangle \equiv \langle K_i^2 \rangle - \langle K_i \rangle^2$,

$$\begin{aligned} \langle \delta K_i^2 \rangle &= \frac{2(N-1)}{N^2(N+1)} \left[\left(\frac{n}{n+2} \right) E \right]^2, \\ &\approx \frac{2}{N^2} \left[\left(\frac{n}{n+2} \right) E \right]^2, \end{aligned} \quad (9)$$

which increases to the hard-sphere limit with larger n , but rapidly decreases with increasing system size.

Finally, the distribution of system kinetic energy is given by the Dirichlet distribution [11], which is a multivariate generalization of the beta distribution and not amenable to visualization or calculation. Alternatively, if we let K_i be independent and identically distributed (i.i.d.) variates drawn from the distributions of either Eq. (7) or (8), then the pdf of $K = \sum_i^N K_i$ can be determined from statistical theory. No such distribution for beta-distributed variates exists for $N > 2$ [18], however, for the gamma distribution, this is $\text{pdf}(K) = \text{G}(N/2, N/(2\langle K \rangle_v); K)$.

Although this has the correct mean, comparison with simulation data shows it has the incorrect variance, and after trial and error, a better approximation was found to be

$$\text{pdf}(K) = \text{G}\left(\frac{n+2}{2}, \frac{N}{2}, \frac{n+2}{2} \frac{N}{2\langle K \rangle_v}; K\right). \quad (10)$$

We justify this distribution not only by the excellent empirical match to the distribution calculated from molecular dynamics (MD) simulation, but also from the connection between the variance of system kinetic energy and the specific heat capacity in the microcanonical ensemble.

In ergodic systems in the thermodynamic limit, Tolman's generalized equipartition theorem [13] applied to Eq. (1) yields an average total energy per grain $\langle \epsilon \rangle = k_B T/2 + k_B T/n$, where k_B is Boltzmann's constant and T is the canonical temperature. The corresponding specific heat per grain is then

$$C_V = \left(\frac{n+2}{2n} \right) k_B, \quad (11)$$

which evidently depends *only* upon the exponent in the potential, i.e., there is no grain material, grain size, or temperature dependence. The equivalence of different statistical ensembles when $N \rightarrow \infty$ implies Eq. (11) is also valid for the microcanonical ensemble in this limit, and when energy is equipartitioned.

It is possible to express the fluctuations in the total system kinetic energy in terms of C_V using the approximation found in Refs. [12,19] which, for 1D systems, is

$$\frac{\langle \delta K^2 \rangle}{\langle K \rangle^2} = \frac{2}{N} \left(1 - \frac{1}{2C_V} \right), \quad (12)$$

where C_V is in units of k_B . Then, using Eq. (11), we have

$$\langle \delta K^2 \rangle = \frac{2}{N} \left(\frac{2}{n+2} \right) \langle K \rangle^2, \quad (13)$$

from which the factor of $(n+2)/2$ appears as part of the distribution variance of Eq. (10).

Equation (12) also provides one method to calculate the specific heat per grain from an MD simulation. However, taking an energy derivative of the so-called microcanonical temperature gives the exact formula for the microcanonical specific heat, which in 1D is [19]

$$C_V = \frac{k_B}{N} \left(1 - \frac{(N-4)\langle 1/K^2 \rangle}{(N-2)\langle 1/K \rangle^2} \right)^{-1}. \quad (14)$$

With this equation and Eq. (10), we can compute an approximate C_V for finite microcanonical systems, via analytic approximations of $\langle 1/K \rangle$ and $\langle 1/K^2 \rangle$ (see the Appendix). The result is

$$C_V = k_B \left[\frac{n+2}{2n} - \frac{1}{N} \left(\frac{n+2}{n} + \frac{4(N-2)}{nN} \right) \right], \quad (15)$$

which has the form of Eq. (11) plus an N -dependent correction term that vanishes in the thermodynamic limit. Hence Eq. (15) provides an estimate for C_V in a large but finite system in which the energy is equipartitioned among the interacting grains.

We point out that all of the distribution functions presented above (per-grain velocity, per-grain kinetic energy, and total system kinetic energy) depend only on the number of grains N , the total system energy E , and, most interestingly, the exponent of the potential energy n .

III. SIMULATION DETAILS

To test the distribution functions in Sec. II, we ran MD simulations of a 1D monatomic chain of N grains held between fixed walls and described by the Hamiltonian in Eq. (1), which includes grain-wall interactions [7]. Our grains and walls are steel, and the grains are 6 mm in radius.

We consider values of the potential exponent n from 2 (harmonic) to 5, and system sizes from $N = 10$ to 100. A standard velocity Verlet algorithm is used to integrate the equations of motion with a 10 ps time step, and no dissipation is included. The grains are set into motion with an initial velocity applied to the first grain only, directed into the chain, causing a SW to propagate through the system. The SW breaks down in collisions with boundaries and in the formation of gaps, creating numerous secondary solitary waves (SSWs). After a

period of time, the number of SSWs increases to a point where the system enters into quasiequilibrium [3,4]. We allow the system to evolve for a substantial amount of time past this phase change, and at least an order of magnitude longer than previous work has considered.

The time scale to equilibrium onset is determined by the potential exponent n [2], so we adjust the velocity perturbation such that the system arrives at equilibrium quickly. Still, it was necessary to collect at least one second of real time data for $n = 2, 2.5, 2.75$, and even longer (up to 6 s) for larger values of n . Data of grain position and velocity are recorded to file every 1 μ s, though we resample the data at time intervals beyond the dampening of velocity autocorrelation (not shown). The deviation from the expected virial $\langle K \rangle_v$ was $< 1\%$ for all systems.

IV. RESULTS AND DISCUSSION

In Fig. 1 we show the distribution functions obtained from MD simulations and the corresponding expected pdfs [Eqs. (5), (7), (8), and (10)] for three representative systems. In each system, the per-grain velocity data agree with the beta distribution, Eq. (5), which is nearly identical to the normal distribution for large N [see Figs. 1(i-a) and 1(ii-a)]. The difference between the normal and beta distributions becomes apparent for small systems ($N \lesssim 30$), where the per-grain velocity data fit the beta distribution better.

The grain kinetic energy distributions are presented in Figs. 1(i-b)–1(iii-b), illustrating agreement between MD results and Eq. (7) for large N . The difference between Eqs. (7) and (8) seems pronounced in the log scale with smaller N , where the beta distribution has a cutoff before the tail of the MD data. However, for $N = 10$, $P(K_i > \langle K \rangle_v) = 0.03\%$, while for larger N it is even less. This shows that the limitation of our original virial approximation is quite small. Finally, the sensitivities to n and N are also shown in Fig. 1, with curves of $n+1$ or $1.1N$. They do not agree as well with the data.

Figures 1(i-c)–1(iii-c) contain the distributions of system kinetic energy from MD simulations, along with the corresponding Eq. (10), for the three systems. The agreement between MD data and the expected result is very good for $N = 100$ [see Fig. 1(i-c)], less so with decreasing N . This is because Eq. (10) develops an increasing skew with decreasing N [cf. Figs. 1(i-c) and 1(iii-c)]. For comparison, we also present the distribution without the variance correction, i.e., $n = 0$, which we call the hard-sphere limit, and clearly does not agree with any MD data of interacting grains.

Lastly, we computed the specific heats of MD simulation data using both Eqs. (12) and (14). These results are directly compared with C_V predicted by Eq. (11) shown as the solid line in both Figs. 2(a) and 2(b), from which it is evident that as N increases, the values calculated by Eq. (12) agree very well with the theory. Moreover, even for small ($N \lesssim 20$) systems, the deviation from theory is no more than $\sim 10\%$ for Eq. (12), and improves with additional statistics. We also present the n, N -dependent C_V predicted by Eq. (15) as dashed lines in Fig. 2(b), which agrees with the MD data within the error bars for $N = 100$.

The fact that the calculated specific heat agrees with the value predicted by the generalized equipartition theorem for

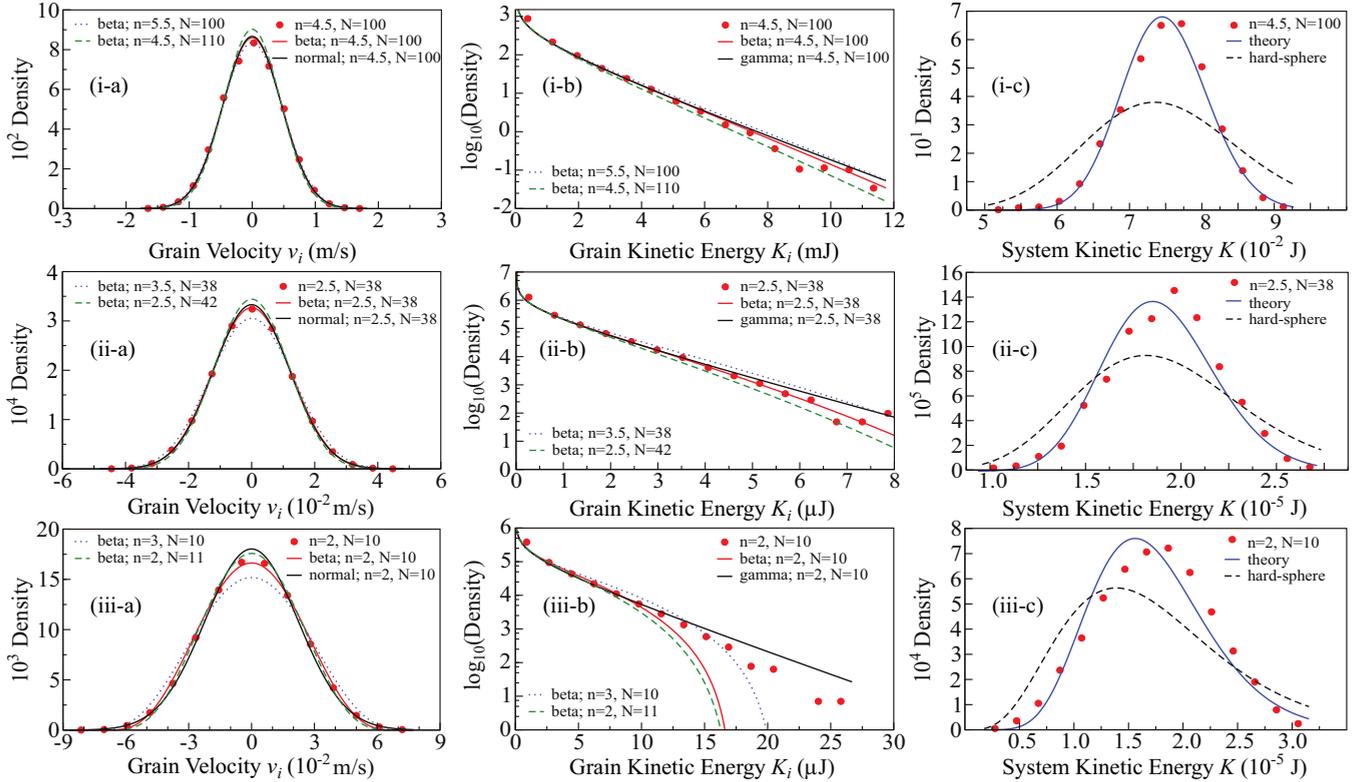


FIG. 1. Distribution of grain velocity, grain kinetic energy, and system kinetic energy for three representative systems. Results of MD simulations are shown as solid circles. In columns (a) and (b), solid lines are predicted distributions [Eqs. (5), (7), and (8)], and dashed-dotted lines are the corresponding distributions with parameters slightly changed to illustrate the sensitivity of Eqs. (5) and (7). In column (c), the solid curve is the theoretical prediction Eq. (10), and the dashed line is the corresponding hard-sphere distribution.

$N \gg 1$ provides evidence that energy is indeed equipartitioned in the Hertz chain at late enough times. Since the dynamics of these systems was previously shown to be ergodic [3], this finally establishes that the very late-time dynamics of 1D granular chains perturbed at one end with zero dissipation is a true equilibrium phase. The appearance of large fluctuations at late times is thus entirely predictable [10]. While real granular alignments are inherently dissipative, dissipation-free versions of our systems may be possibly realized as integrated circuits and hence our results may be observable in the laboratory. Finally, a quantitative analysis of the QEQ phase may now be possible with this equilibrium theory as the starting point.

The caveat to this is that we have considered only asymmetric perturbations. Consider instead a 1D chain of an odd number N of grains that is perturbed by symmetric velocity pulses from both ends. The middle grain would never move, thus kinetic energy could not be equipartitioned among all the grains. However, due to the symmetry of the system, in a sense the left $(N - 1)/2$ and the right $(N - 1)/2$ grains are nothing more than separate subsystems that have been perturbed asymmetrically. Hence energy will be equipartitioned in each of these two subsystems as $t \rightarrow \infty$, and their late-time dynamics will be described by equilibrium statistical mechanics. This implies that energy is equipartitioned among the available degrees of freedom in Hertz systems at long times. This ultimately has an impact on the microcanonical distribution functions and the specific heat, which is further explored below.

Symmetrically perturbed systems

The number of independent degrees of freedom in Hertz systems can be reduced by imposing periodic boundary conditions [17], or by symmetrically perturbing the system (velocity perturbations at both chain ends of equal magnitude, directed into the chain). Perturbing the system in this way results in a mirror-reflection symmetry to be induced in the system, thus halving the degrees of freedom, and in turn affecting the probability distribution functions and specific heat capacity.

Because every grain can still individually visit the same total phase space volume with the same probability as computed earlier, the distributions of grain velocity and grain kinetic energy are independent of the degrees of freedom and are still given by Eqs. (5) and (7) [and Eq. (8)]. Since N grains were used to compute the normalized histogram, N is used for the distribution function parameters.

However, the distribution of system kinetic energy, Eq. (10), must be modified to account for the loss in the number of degrees of freedom due to the resulting spatial symmetry. This is because Eq. (10) was derived from statistical theory under the assumption of drawing N identical and independent random variates (grain kinetic energies) from a gamma distribution; however, by perturbing the system symmetrically, this is no longer the case.

In particular, due to the mirror reflection symmetry about the center of the chain, a system with even N loses $N/2$ degrees of freedom from the momentum (and $N/2$ from

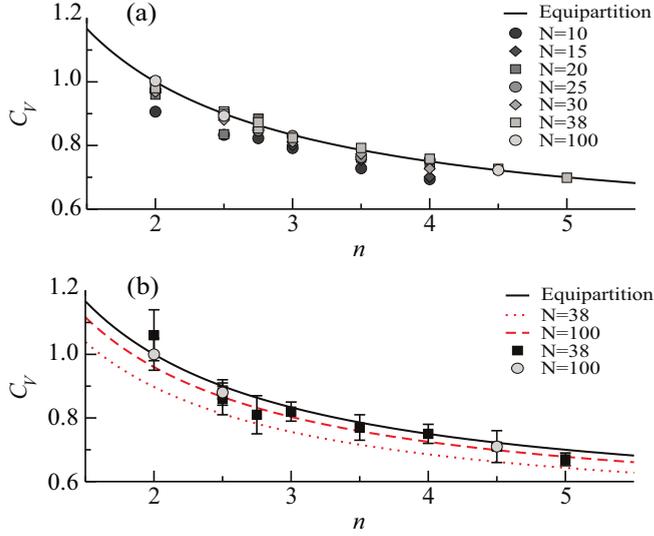
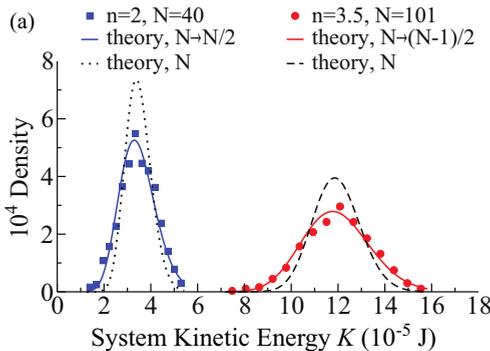


FIG. 2. Specific heat capacities (in units of k_B) computed for all MD simulated systems as a function of the exponent on the potential. In (a) we present values obtained from inverting Eq. (12), and in (b) values obtained from Eq. (14). The solid line in both plots is the specific heat predicted by the generalized equipartition theorem, Eq. (11). The dashed lines in (b) are specific heats predicted by Eq. (15).

the grain positions). Hence there are *only* $N/2$ independent grain kinetic energies in such systems. Similarly, in a system with odd N , $(N-1)/2$ degrees of freedom are lost from the momentum [and $(N-1)/2$ from position], as well as an additional two degrees of freedom (one from momentum, one from position) since the central grain never moves when the system is perturbed symmetrically. Thus *only* $(N-1)/2$ of the grain kinetic energies are independent in odd- N systems. The approximate distribution function for the system kinetic energy in such systems is then given by Eq. (10), after replacing N with the number of independent grain kinetic energies,



i.e., $N \rightarrow N/2$ for even N and $N \rightarrow (N-1)/2$ for odd N , and with E the total energy of the system. We illustrate the agreement between these distribution functions and MD data for both an even- N and an odd- N representative system in Fig. 3(a).

Finally, since the specific heat is connected to the fluctuations in the system kinetic energy, it is expected that the microcanonical specific heat should also be modified. The previous Eq. (14) gives nonsensical and negative values of C_V for the symmetrically perturbed cases, since it is based on the assumption of N total degrees of freedom of momentum. The correct expression for the modified specific heat was derived previously [20], and for even- N systems it is

$$C_{V,\text{even}} = \frac{2k_B}{N} \left(1 - \frac{(N-8) \langle 1/K^2 \rangle}{(N-4) \langle 1/K \rangle^2} \right)^{-1}, \quad (16)$$

and for odd- N systems it is

$$C_{V,\text{odd}} = \frac{2k_B}{(N-1)} \left(1 - \frac{(N-9) \langle 1/K^2 \rangle}{(N-5) \langle 1/K \rangle^2} \right)^{-1}. \quad (17)$$

Proceeding in an identical fashion to that of Ref. [19], one can obtain approximate expressions relating the above two formulas for C_V to the system kinetic energy fluctuations. Setting $K = \langle K \rangle + \delta K$ and expanding $1/K$ in a Taylor series, retaining only terms to order N^{-1} , the resulting expressions are analogous to Eq. (12), except appropriately modified to account for the spatial symmetry of the system. The result is

$$\frac{\langle \delta K^2 \rangle}{\langle K \rangle^2} = \frac{4}{N} \left(1 - \frac{1}{2C_{V,\text{even}}} \right) \quad (18)$$

for even- N systems, and

$$\frac{\langle \delta K^2 \rangle}{\langle K \rangle^2} = \frac{4}{N} \left(1 - \frac{N}{2(N-1)C_{V,\text{odd}}} \right) \quad (19)$$

for odd- N systems. Note that in both Eqs. (18) and (19), C_V is in units of k_B .

While these equations seem little changed from earlier equations with full degrees of freedom, Eqs. (12) and (15),

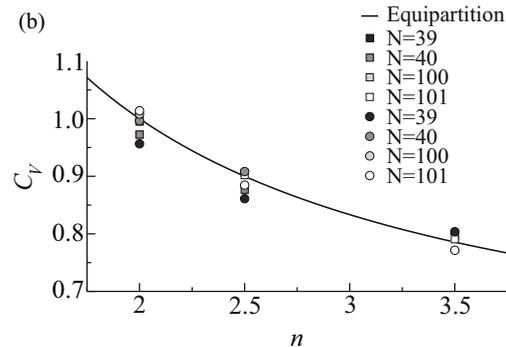


FIG. 3. Results of chains with even and odd N , perturbed by symmetric velocity perturbations. (a) Distribution of system kinetic energies for an $n = 2$, $N = 40$ system and an $n = 3.5$, $N = 101$ system. Data for the second system were scaled by 10^{-3} in the x domain and 10^3 in the y domain to fit in the viewport. Results of MD simulations are shown as solid symbols. Dashed-dotted lines are the predicted distributions [Eq. (10)], and solid lines are the predicted distributions [Eq. (10)] with the symmetrically imposed reduced degrees of freedom, i.e., with $N \rightarrow N/2$ for even N , and $N \rightarrow (N-1)/2$ for odd N . (b) Specific heat capacities computed for all symmetrically perturbed MD simulated systems as a function of the exponent on the potential. Circles correspond to values obtained from Eqs. (16) and (17), and squares correspond to values obtained from inverting Eqs. (18) and (19). The solid line is the specific heat predicted by the generalized equipartition theorem, Eq. (11).

only these give the correct result as seen in Fig. 3(b), where we show the resulting heat capacities calculated using both Eqs. (16) and (18) for a representative even- N system, and Eqs. (17) and (19) for a representative odd- N system, which have been perturbed symmetrically at both ends.

It is clear from Fig. 3(b) that the calculated specific heats agree well with the values predicted by the equipartition theorem, Eq. (11), indicating that energy is also shared equally in symmetrically perturbed systems. Since this is the case even for odd- N systems, where the central grain never moves, the definition of “equipartitioning of energy” must be clearly defined in such systems. While energy equipartitioning is sometimes erroneously discussed in terms of energy being shared equally among all particles in a system, the equipartition theorem makes no reference to particles, but rather to the independent degrees of freedom in a system [21]. Hence the fact that the specific heat per particle, Eqs. (16) and (17), agrees with the value predicted by the equipartition theorem implies that the energy is being spread out equally over all the *independent degrees of freedom* at long times in Hertzian chains.

V. CONCLUSIONS

Here we have shown that the long-term dynamics of Hertz chains is described by a microcanonical ensemble of interacting particles. As demonstrated by the calculated heat capacity, energy equipartitioning occurs in such systems, indicating that their long-term fate is indeed an equilibrium phase.

These results are also an empirical demonstration of how the potential energy function can affect the kinetic energy distribution. Shirts *et al.* [17], in their calculation of the exact distribution for the finite hard-sphere system, speculate that for attractive potentials $\text{pdf}(K_i)$ would differ somehow, but concede it would be exceedingly complicated to derive. We have shown accurate distributions that may guide attempts to solve Eq. (3) for finite interaction potentials.

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APPENDIX

The cumulative distribution function of K is $F_K(K_0) \equiv P(K < K_0)$. Now consider $X \equiv K^{-\rho}$, where $\rho > 0$. By definition, $K \geq 0$, thus $F_X(x) = 0$ for $x < 0$. Meanwhile for $x > 0$, $F_X(x) \equiv P(0 < K^{-\rho} \leq x) = P(K \geq x^{-1/\rho}) = 1 - P(K < x^{-1/\rho}) = 1 - F_K(x^{-1/\rho})$. The $\text{pdf}(X)$ is given by $dF_X(x)/dx$, thus $\text{pdf}(X) = F'_K(x^{-1/\rho})/(\rho x^{(\rho+1)/\rho}) = [\text{pdf}(K)]_{k=x^{-1/\rho}}/(\rho x^{(\rho+1)/\rho})$. Knowing the pdfs of $1/K$ ($\rho = 1$) and $1/K^2$ ($\rho = 2$), the means $\langle 1/K \rangle$ and $\langle 1/K^2 \rangle$ can be computed in a standard way.

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